Quantum and Dirac Materials for Energy Applications Conference,
Santa Fe, March 8-11th, 2015

Research on Materials for Nuclear Energy Technology at the Royal Institute of Technology - KTH
+
Educational activities

Waclaw Gudowski

In collaboration with: Sevostian Bechta, Janne Wallenius, Pär Olsson, Mikael Jolkkonen + more

Reactor Physics, KTH

Stockholm

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We have very solid foundations for a good KTH-LANL cooperation starting from 1992 (without any MoU's)

- Saltsjöbadet Conference – 1992. First US-Russia meeting of weapon scientists!
- Co-organizing I, II, III International ATW Conferences
- Establishment of ISTC – Swedish membership of ISTC
- 1 MW spallation target and opening of heavy metal coolant technology (Trento Workshop 1997). European start of this technology!
- A lot of student PhD exchange until 2001
- Co-director of ISTC 2006-2011– work with Anne Harríngton, Steve Gitomer, Glenn Schweitzer, R. Lehman II. Housing Lab2Lab cooperation meetings etc.

OUTLINE

- Organisation
- Education
- Research:
  - Materials for energy technology
  - Computer simulations in materials for nuclear energy technology
- Summer Course on Geological Storage of Spent Nuclear Fuel
- Cooperation strategy

Organisation

3 (Sub-)departments at School od Engineering Sciences:

- Nuclear and Reactor Physics
- Nuclear Power Safety
- Reactor Technology

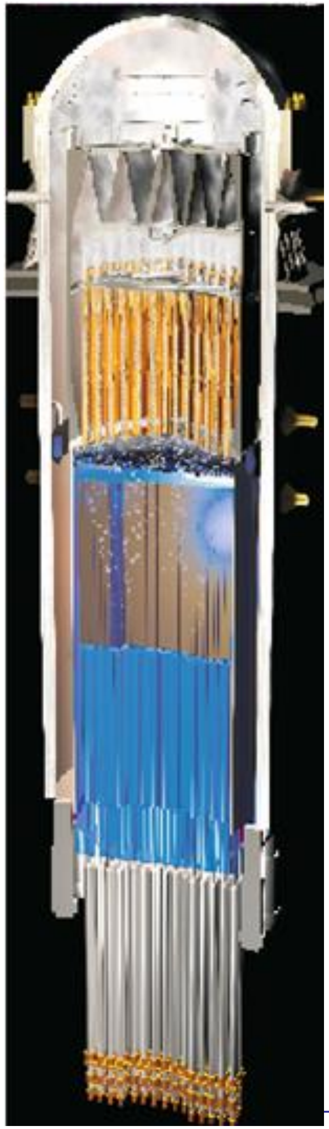
In other schools:

- Nuclear Chemistry
- Nuclear material mechanics
- Nuclear safety philosophy
- R&D activities at Material science, Surface & corrosion science

Master programme in nuclear energy engineering

- Major joint effort
- Two year program focused on fission power engineering
- Started in 2007
- About 30 students annually
- **Major courses attended by > 40 students**
- Most senior scientists involved in teaching
- Emphasis on nuclear power safety, advanced nuclear and nuclear waste management (back-end of the nuclear fuel cycle) and Gen IV reactors
- Dual Diploma program in the European Master in **Innovative** Nuclear Energy – EMINE, DD agreements with Tsnighua University, KAIST etc.
- Program director : Waclaw Gudowski

KTH covers all important aspects of nuclear technology today and in the future

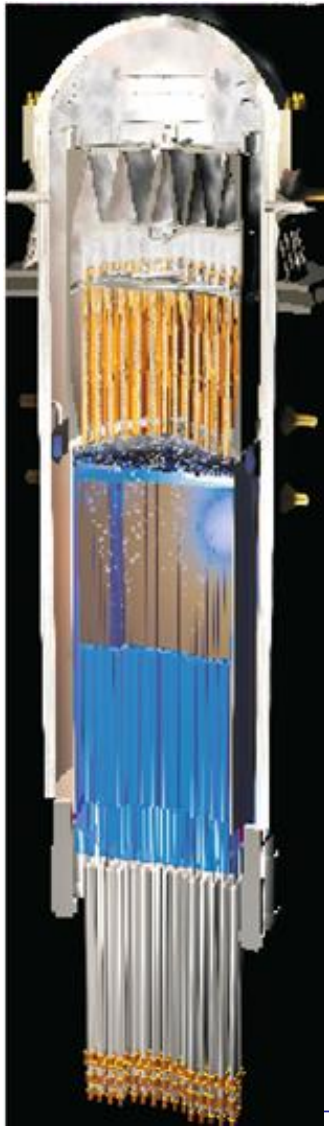


Nuclear Power Safety – ”keeping heat under control”
- o Research on inherent safety mechanisms and safety analysis
- o Severe accident research and management
- o Heavy metal and sodium fast reactor safety – **Gen IV research**

Reactor Technology – **”keeping boiling under control”**
- o Thermal hydraulics of Light Water Reactors
- o 2-phase flow, boiling and dry-out processes
- o Uprating and life extension of reactors

Reactor Physics – **”keeping neutrons and wastes under control”**
- o **Gen IV concepts and transmutation of nuclear wastes-ADS**
- o New nuclear fuels
- o Materials in radiation environment
- o Safety limits in reactor kinetics etc.

KTH covers all important aspects of nuclear technology today and in the future



Nuclear Chemistry – **”keeping nuclear waste and reactor chemistry under control”**

- Radionuclides in a repository for spent reactor fuel
- Experiments both in-situ in “real boreholes” in Äspö geological repository laboratory and in a chemical laboratories at KTH

Material sciences – **”keeping ageing and radiation damage under control”**

- Radiation damage in materials
- Ageing of materials
- Simulation of material in radiation environment, Monte Carlo and Molecular Dynamics

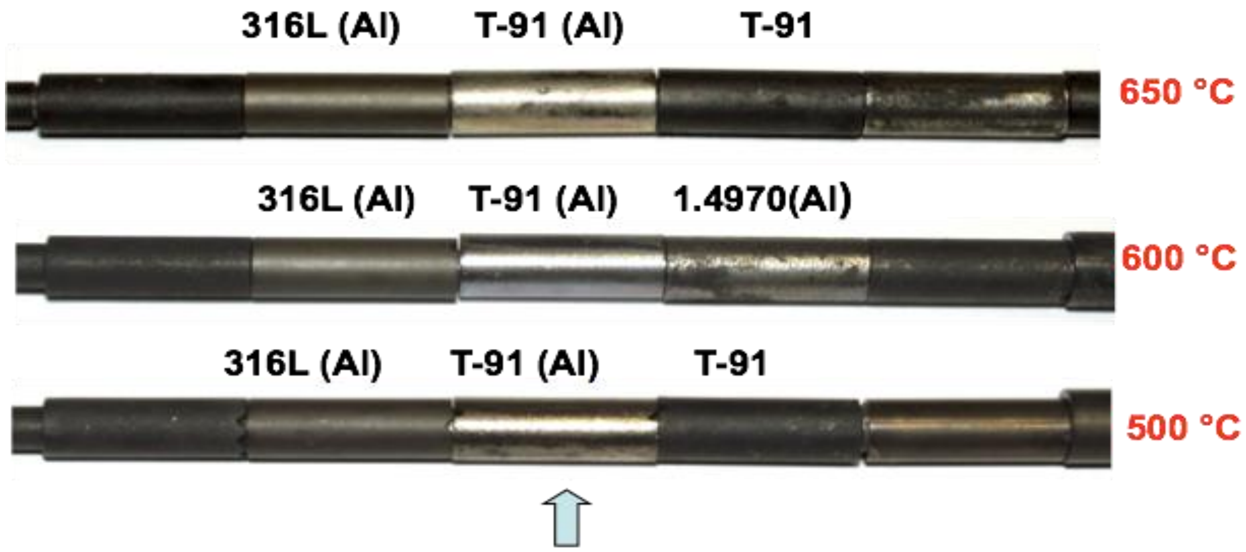
Research towards heavy metal coolant (Pb – Pb/Bi) - corrosion in lead

Research towards heavy metal coolant - corrosion in lead

- Russian ferritic-martensitic steel EP823 (2% Si) after 16 000 h in flowing lead at 650°C (~2 ppm oxygen)
- 30 000 h tests at 600°C show equally good performance

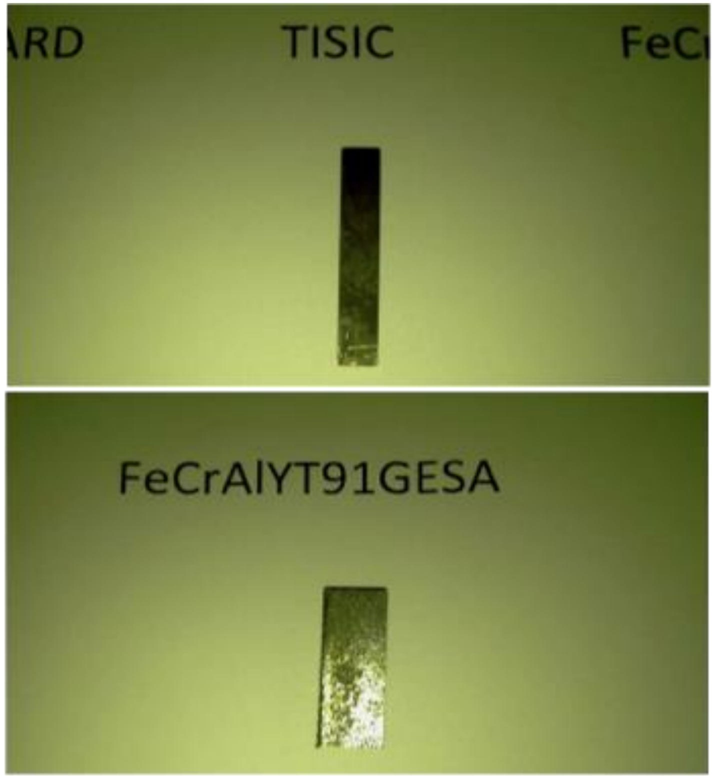
Research towards heavy metal coolant - corrosion in lead and alumina protection

- 1500 h corrosion test in flowing liquid lead at 50 ppm oxygen



- GESA treated T91 in perfect condition after > 17 000 h at 550°C

Research towards heavy metal coolant - possible solutions



- MAXTHAL (TiSiC)
- FeCrAlY
- Both materials are fabricated by Sandvik!

A unique experimental facility: Pb/Bi loop for heavy metat coolant and natural convection studies - TALL-3D

A Thermal-hydrAulics LBE Loop with 3D test section (TALL-3D) for validation of multi-scale and coupled codes: System Thermal-Hydraulics (STH) and Computational Fluid Dynamics (CFD) codes.

TALL-3D - a 5.8 meters high liquid lead-bismuth eutectic (LBE) loop consisting of three parallel vertical legs.

The main heater leg (left) has a rod type heater in its lower part. The main heater is essentially an electrically heated rod co-axially inside a pipe at the lower part of the main heater leg. Rod heater is 8.2 mm in diameter and the heated part has a length of 870 mm. Top of the main heater leg accommodates an expansion tank. The 3D leg (middle) has a heated pool type test section in its lower part and the heat exchanger (HX) leg (right) has a heat exchanger in the top part and an electric permanent magnet (EPM) pump below it.

Lead-bismuth is stored in a sump connected to the lower left corner of the loop.

The KTH Nuclear Fuel Laboratory

Dr. Mikael Jolkkonen, Dept. of Reactor Physics, KTH, Stockholm

History of the KTH Fuel Lab

2015 First uranium silicides produced

First uranium carbides produced

2014

New analytical section of laboratory operational

2013

Real-time MS monitoring of processes is introduced

2012

Laboratory space is again doubled

2011 Spark-plasma sintering introduced as standard method

Laboratory space is doubled

2010

First UN pellets produced(conventional sintering)

2009

First uranium nitrides produced

2008

Test runs of synthesis equipment with zirconium nitrides

2007

Construction of lab starts

2006 Decision to establish lab - search for funding

Nitride fuels

Already before year 2000, the Department of Reactor Physics had a particular interest in nitride fuels for fast reactors and ADS. We collaborated in a production campaign (CONFIRM) in Switzerland, but had no facilities for nitride production in Stockholm (or anywhere else in Sweden).

Today there are two nitride fuel production laboratories in Sweden, one at KTH, the other at Chalmers (in Gothenburg).

Sintering (SPS)

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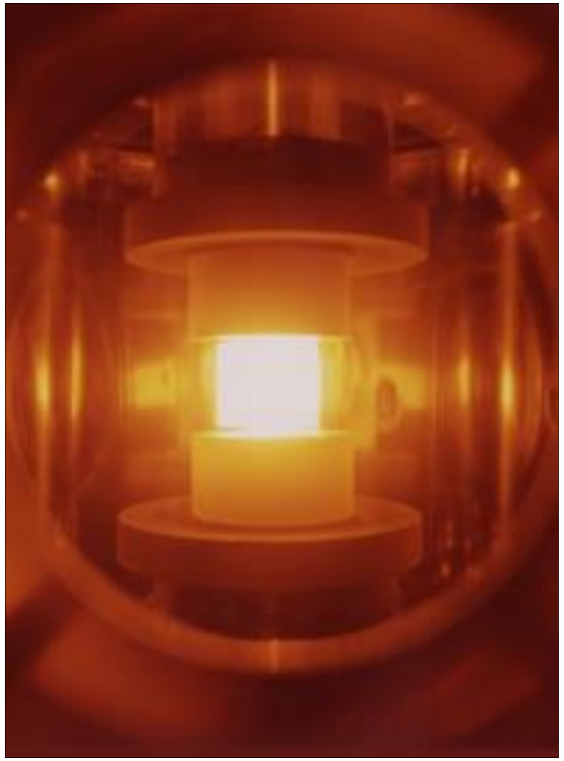
Using spark-plasma sintering, uranium nitride pellets of a density exceeding 99 %TD have been produced at KTH. The temperatures needed are low (≈ 1550 °C) and sintering time is short (3 - 10 min).



UN pellet
furnace
pellet

SPS
ZrN

^{15}N enriched nitride fuels

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- It is commonly expected that nitride fuels will be manufactured with ^{15}N to improve neutron economy and to avoid large amounts of ^{14}C in the reprocessing stream.
- To limit the manufacturing costs, it is necessary that neither synthesis nor reprocessing leads to waste of ^{15}N.
- Methods to conserve nitrogen at both ends of the fuel cycle have been experimentally demonstrated at the KTH Nuclear Fuel Lab.

Image: Hydriding/nitriding furnace during high-temperature de-nitriding of U_2N_3 to UN.

Nitrides in LWR

- A rapidly increasing interest for nitride (and silicide) fuels for LWR applications can be noted
- We have since 2011 been looking at methods to increase UN resistance in water/steam environments
- Early experiments in uninstrumented pressure capsules confirmed serious attack above 300 °C
- Admixture of ZrN in solid solution did not significantly improve the resistance of the pellets
- Instead, it was found that differences in raw material quality, and in particular the sintering conditions, had a strong influence.

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UN testing in superheated steam

- Decomposition by hydrolysis:
  $UN + 2\ H_2O \rightarrow UO_2 + NH_3 + 1/2\ H_2$
- Steam flow controlled by LKB HPLC pump (10 - 9999 µl/min) (water feed to internal capillary steam generator)
- Atmosphere mix controlled by Bronkhorst flow regulators (argon flow rate)
- Ammonia collected in wash bottle (with dilute H_2SO_4)
- H_2 production monitored in real-time by MS (Hiden QGA)
- Temperature monitored at two points with external TC

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Reprocessing studies of UN

- No difficulties have been encountered in acid dissolution of dense *unirradiated* UN pellets in nitric acid. Neither elevated temperatures nor any additives appear to be needed.
- It has not been tested at our laboratory whether isotopic dilusion of ^{15}N would occur in such dissolution. In any case, it would be an advantage if no nitrates were introduced in the stream.
- The controlled decomposition, at moderate temperatures, of UN into ammonia and a dry oxide powder offers a convenient way to recover ^{15}N from nuclear fuel manufactured with enriched nitrogen.
- MS measurements of uncondensed steam exhaust show that N_2 and NO_x are not formed, except under exceptionally high hydrolysis rates more resembling combustion in steam.
- The recovered ^{15}N ammonia is a suitable reactant for synthesis of nitrides from metals or halide salts.

Uranium silicides

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- Uranium silicides such as U_3Si_2 and (approximately) U_3Si_5 are potentially useful fuel materials in themselves.
- We are at the present time more interested in modifying the properties of UN by addition of a second silicide phase.
- Our observations are that silicide addition permits the manufacture of exceptionally dense nitride pellets.
- Upcoming experiments will show what effect the additive has on the resistance to oxidation and hydrolysis of pellets.

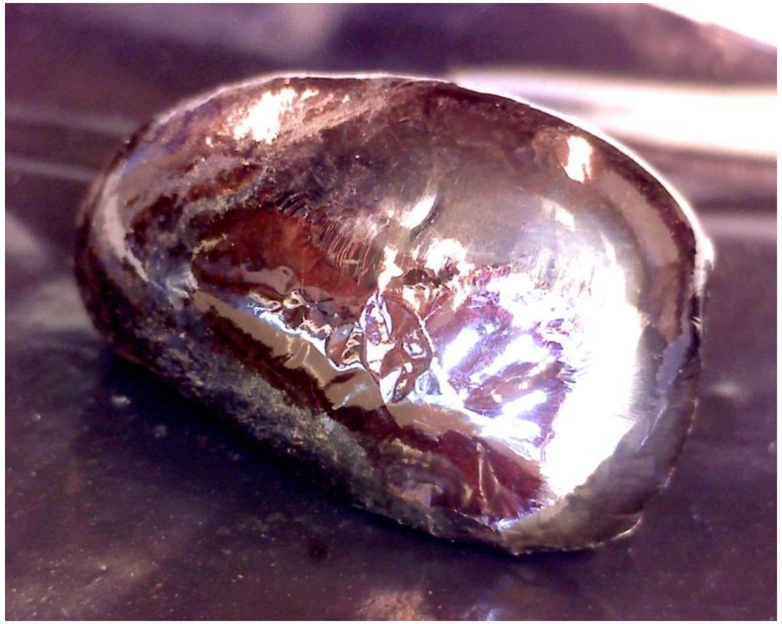
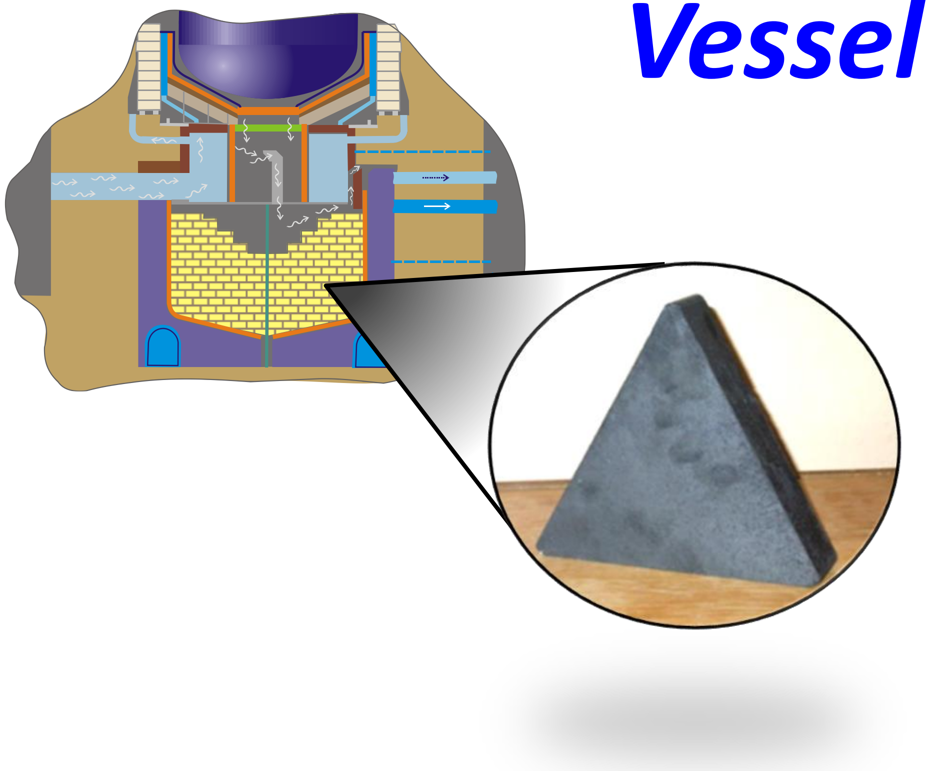
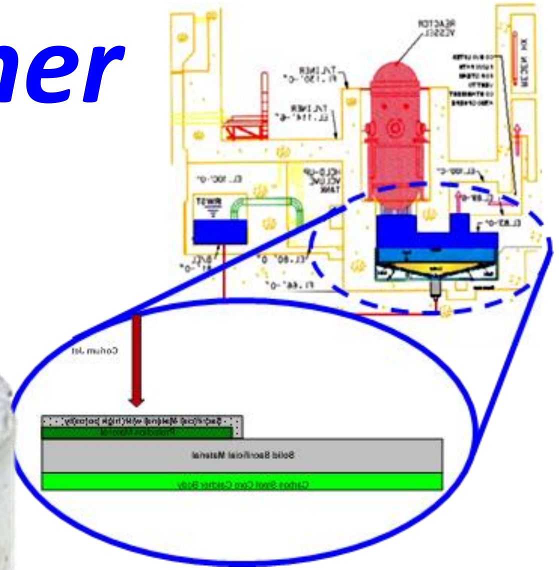


Image: U_3Si_2 produced at KTH.

New Reactor Functional Materials: Sacrificial Materials of the Ex-Vessel Core Catcher





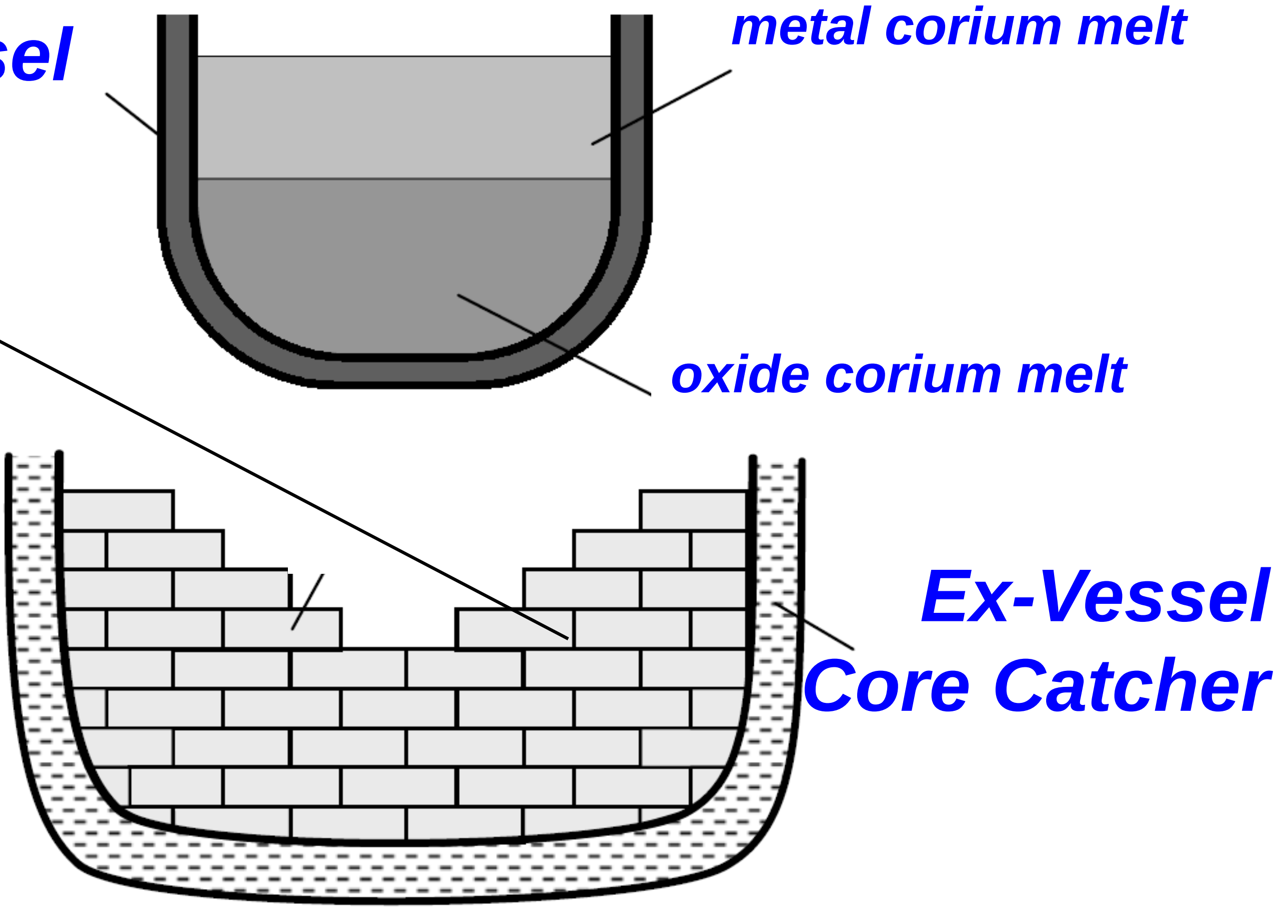
Andrei Komlev, Sevostian Bechta and **Waclaw Gudowski**

Idea of Sacrificial Material (SM)

- ✓ *It is complicated to manage melt properties at IVR but we can do it during ex-vessel melt stabilization*

Sacrificial material:

- ✓ *Oxidic to dilute UO_2-ZrO_2-Zr melt*
- ✓ *Steel to dilute Fe – Cr-Ni-U-Zr (O) melt*



SM compositional alternatives

Metal SM

Marked decline of overheating metallic melt temperature

Fe

Economic

Decreasing of generation density in metallic melt after inversion

Interaction of steel with metal and corium melts is well investigated

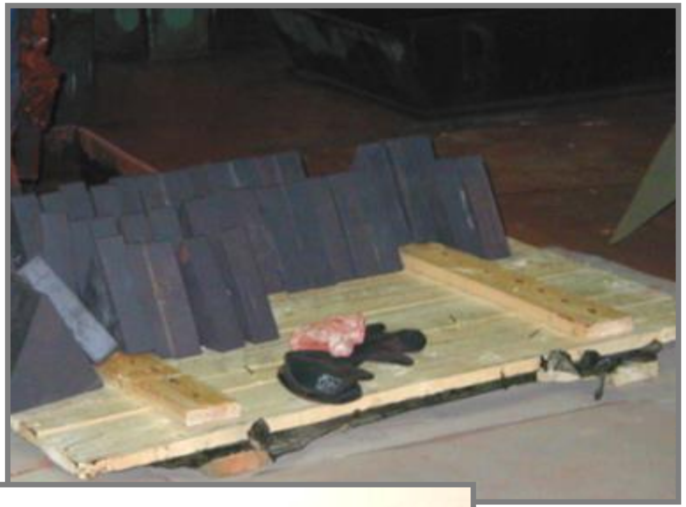
Oxide SM

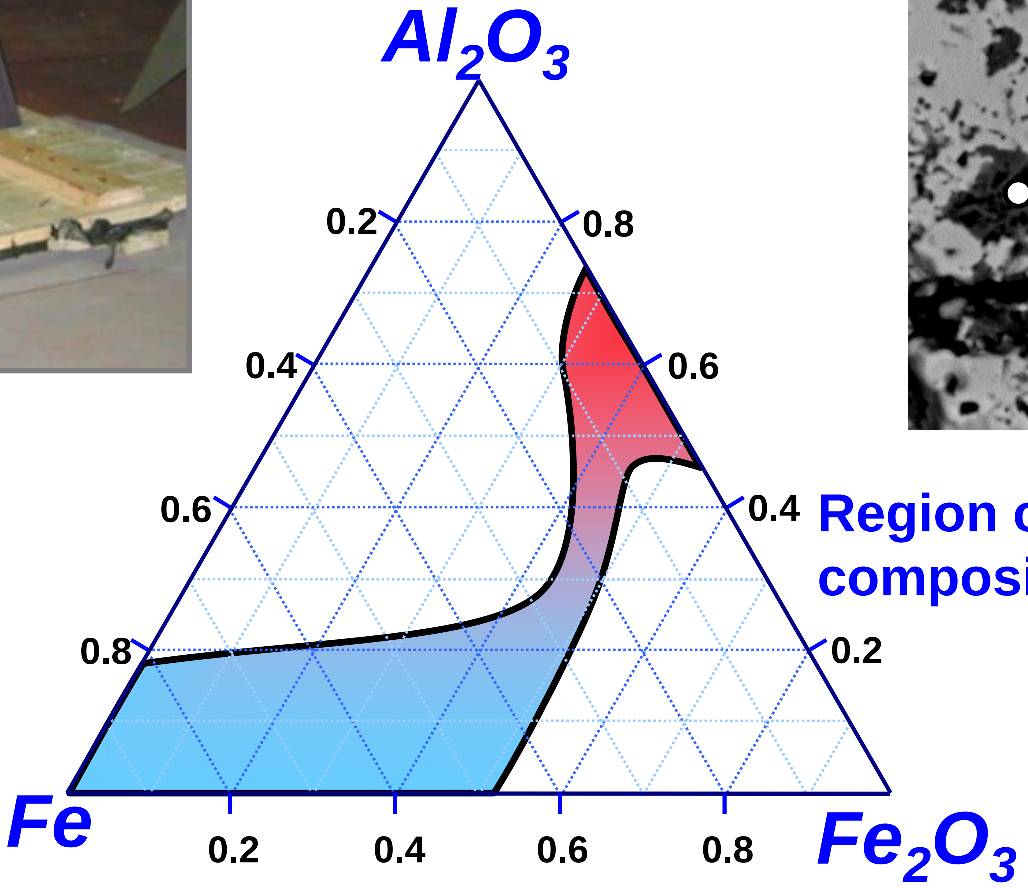
Oxide properties being criteria for choice of sacrificial material

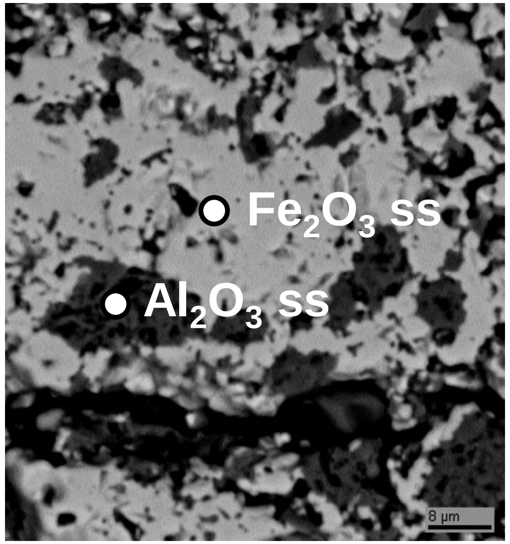
Oxide	ρ_{melt}, $^{kg}/_{m3}$	T_{melt}, °C	Q_{melt}, $^{MJ}/_{kg}$	C_p, $^{kJ}/_{kg\ K}$	Degree of investigation of interaction with corium
MgO	3020	2826	1.93	0.93	Poor
Al_2O_3	3050	2053	1.09	0.77	Well
SiO_2	2390	1722	0.16	0.74	Well
CaO	3220	2626	0.93	0.75	Poor
Sc_2O_3	3470	2488	0.92	0.68	Poor
TiO_2	4000	1911	0.85	0.69	Poor
Cr_2O_3	4690	2431	0.82	0.79	Poor
Fe_2O_3	4730	1538	0.59	0.65	Well
Fe_3O_4	4850	1596	0.59	0.65	Well
SrO	4230	2656	0.67	0.43	Well
ZrO_2	5150	2709	0.73	0.46	Well
BaO	5150	2016	0.39	0.31	Poor

Determination of SM integral composition

Results of studies in 1999-2001



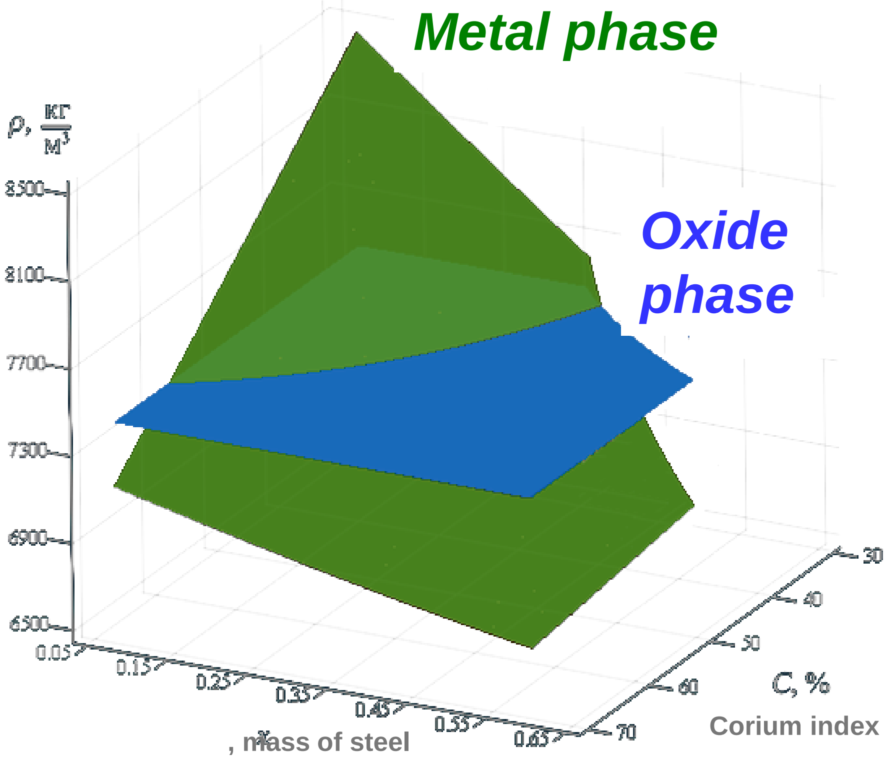


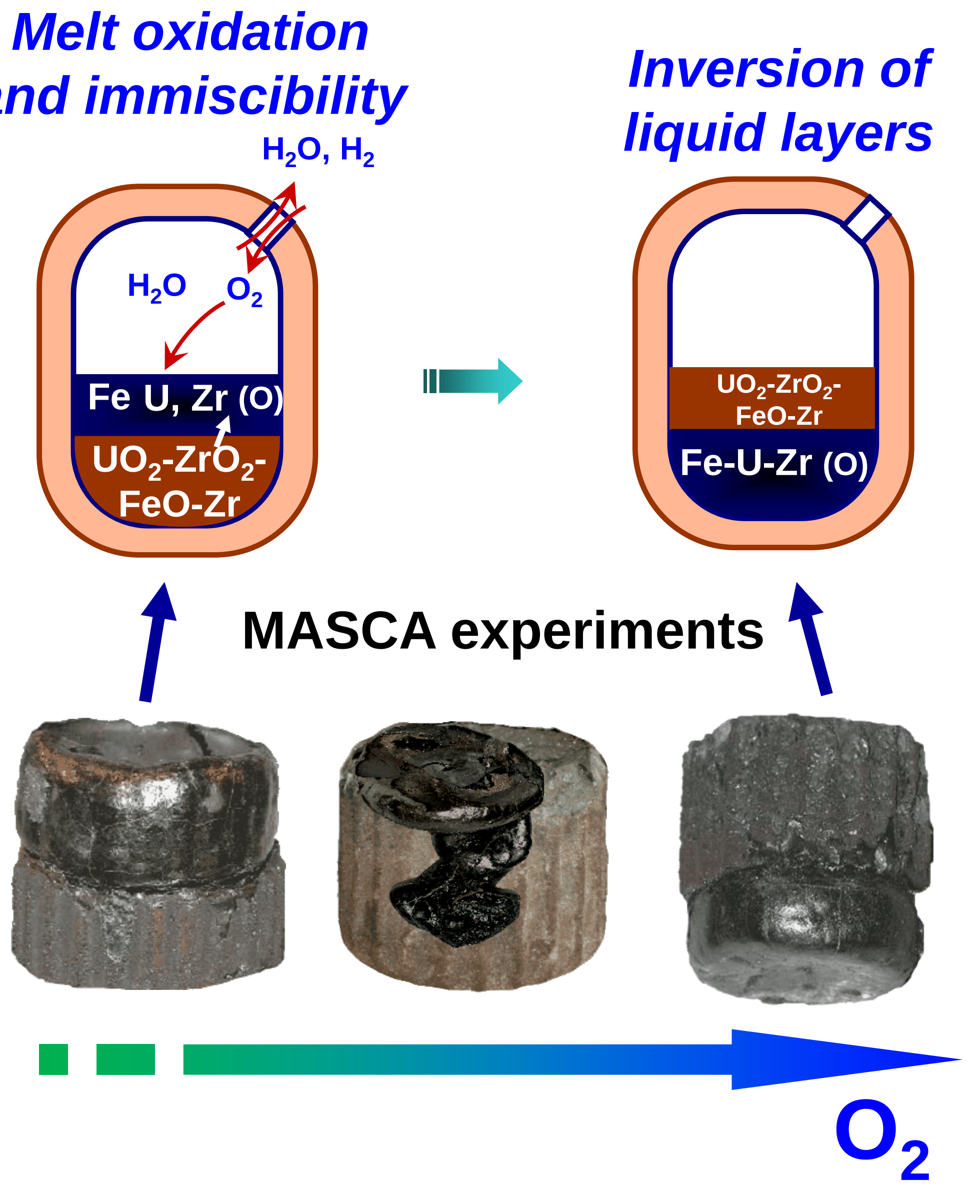


Region of preferable compositions

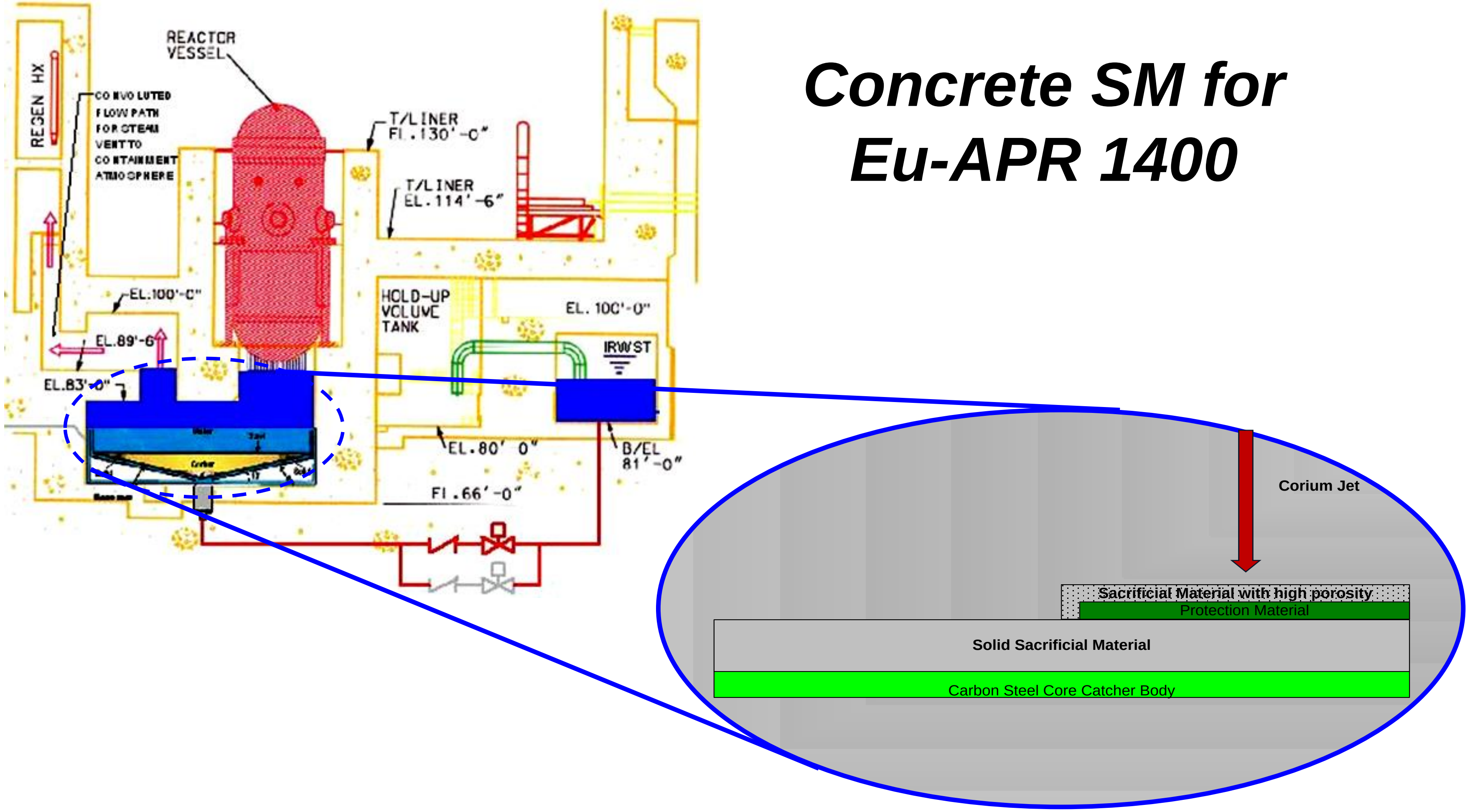
+ Micro-components: SrO, Gd_2O_3

Physicochemical phenomena in corium molten pool





Sacrificial Concretes: New developments

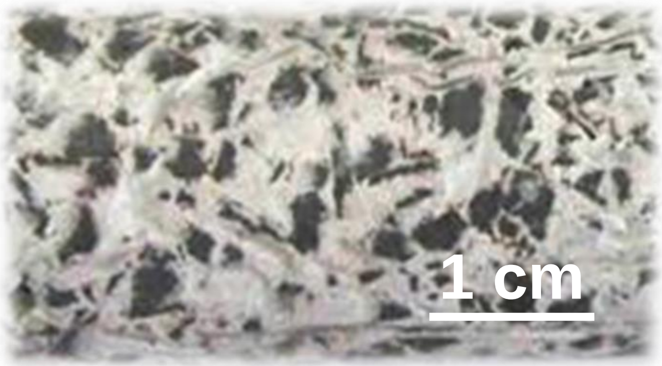


Concrete SM for Eu-APR 1400

Korean partners: KHNP, KEPCO and KAERI

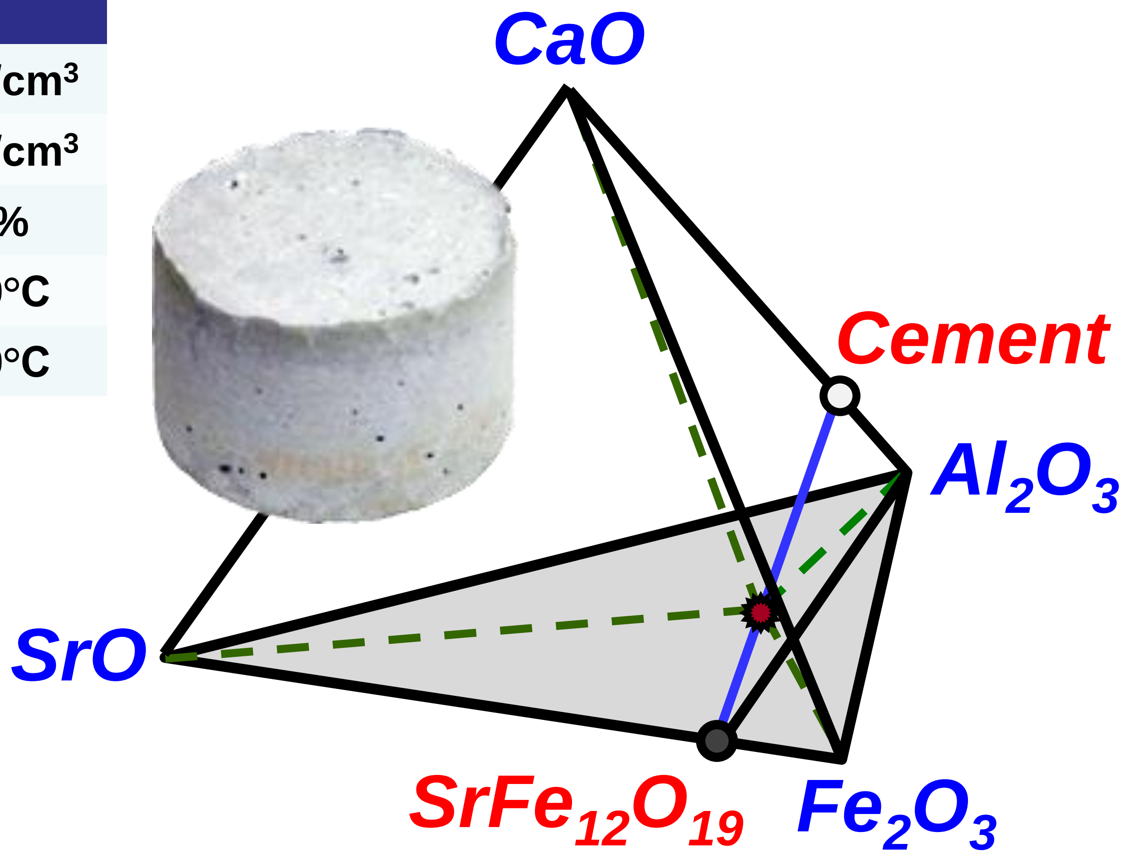
Sacrificial concrete with Strontium hexaferrite

Property	Value
Apparent density	2.4–3.3 g/cm³
Pycnometric density	4.4–4.6 g/cm³
Porosity	30–50 %
Solidus temperature	1405±10°C
Liquidus Temperature	1610±20°C



material macrostructure

Results of investigations 2010-2011



Future priorities: Material Physicochemical Design

Hierarchical levels

Requirements

Chemical compound	Isotope, Element
Substances	Chemical composition, Phase state
Materials	Phase composition, microstructure macrostructure
Wares	Shape, size
Construction	Connectivity type

Capabilities

Acknowledgements to our partners

Saint-Petersburg State Institute of Technology

Saint Petersburg Electrotechnical University

ATOMPROEKT (AEP)
Enterprise of ROSATOM State Corporation

Research Institute of Technology of ROSATOM (NITI)

Royal Institute of Technology (KTH)

Computer simulations of materials for nuclear energy technology

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Diffusion controlled phenomena in materials for nuclear energy technology

Pär Olsson[a], Luca Messina[a], Zhongwen Chang[a], Antoine Claisse[a]

Maylise Nastar[b],Thomas Garnier[b], Christophe Domain[c], Oscar Grånäs[d], Igor di Marco[d], Marco Klipfel[b], Paul van Uffelen[e], Pål Efsing[f], Dmitry Terentyev[g], Giovanni Bonny[g], Lorenzo Malerba[g], Charlotte Beqcuart[h]

Contact: polsson@kth.se

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Main topics

1. Diffusion in nitride fuels

2. Embrittlement and radiation induced segregation in ferritic steels

3. Swelling in bcc and fcc materials

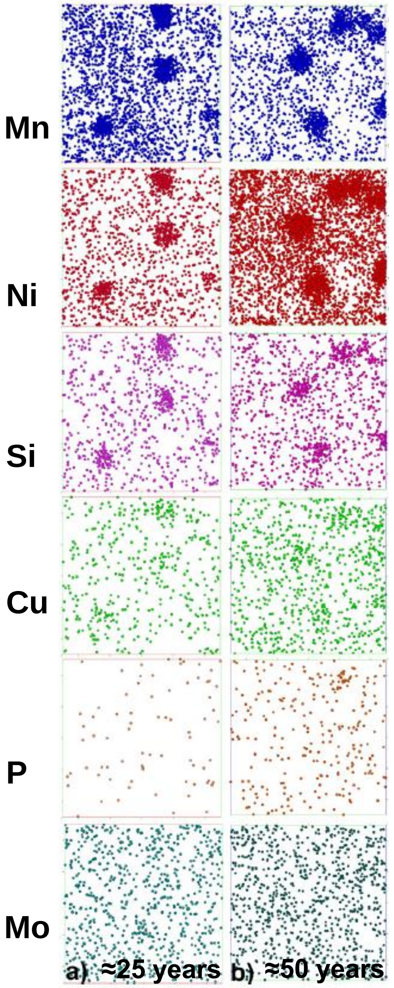
Status of nitride modeling

- New FGR (Fission Gas Release) models in TRANSURANUS, applicable to nitrides, oxides, ...

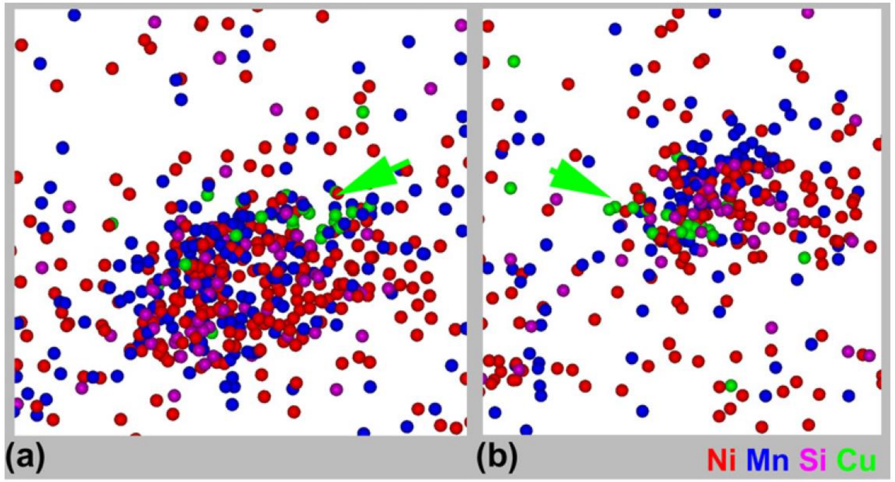
- Ab initio study of self- and impurity diffusion in UN and (Pu,U)N

2 – Embrittlement in RPV steels

Atom maps (R4)



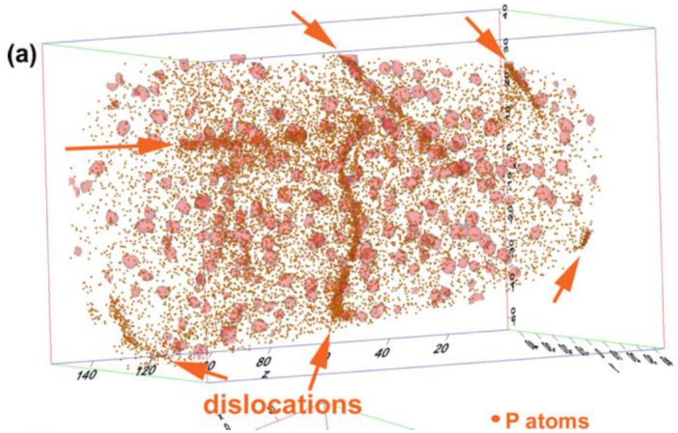
Mn-Ni-(Si)-(Cu) nanocluster (R3)



Miller et al., JNM 437 (2013)

Ringhals surveillance capsules
(atom probe tomography)

P segregation to dislocations (R4)

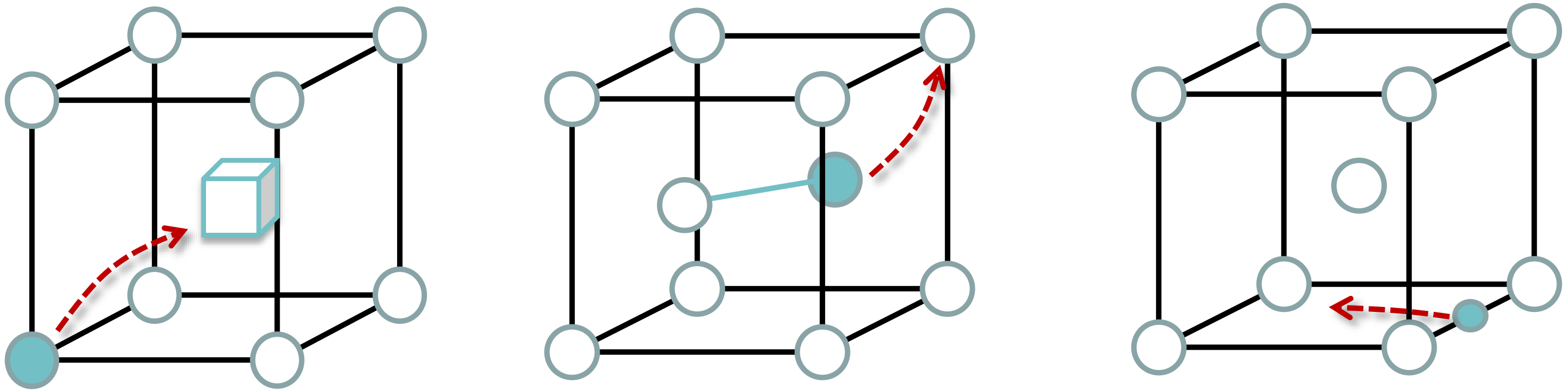


(radiation-induced)

Cu-rich precipitates

(radiation-enhanced)

Solute diffusion in alloys



Vacancy exchange   Dumbbell migration   Foreign interstitial

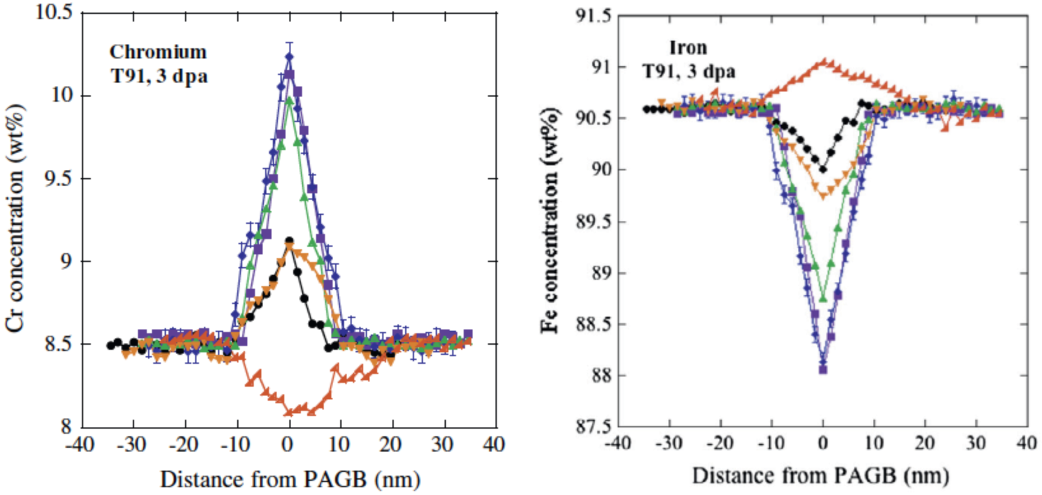
Diffusion capability depends on:

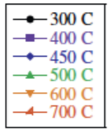
- Stability of the defected configuration (binding energies).
- Transition (jump) rates.

$$P_{config} \propto \exp\left(\frac{-E^{B}_{config}}{k_B T}\right) \qquad \omega = \nu \exp\left(-\frac{E^{M}}{k_B T}\right)$$

Radiation-induced segregation (RIS)

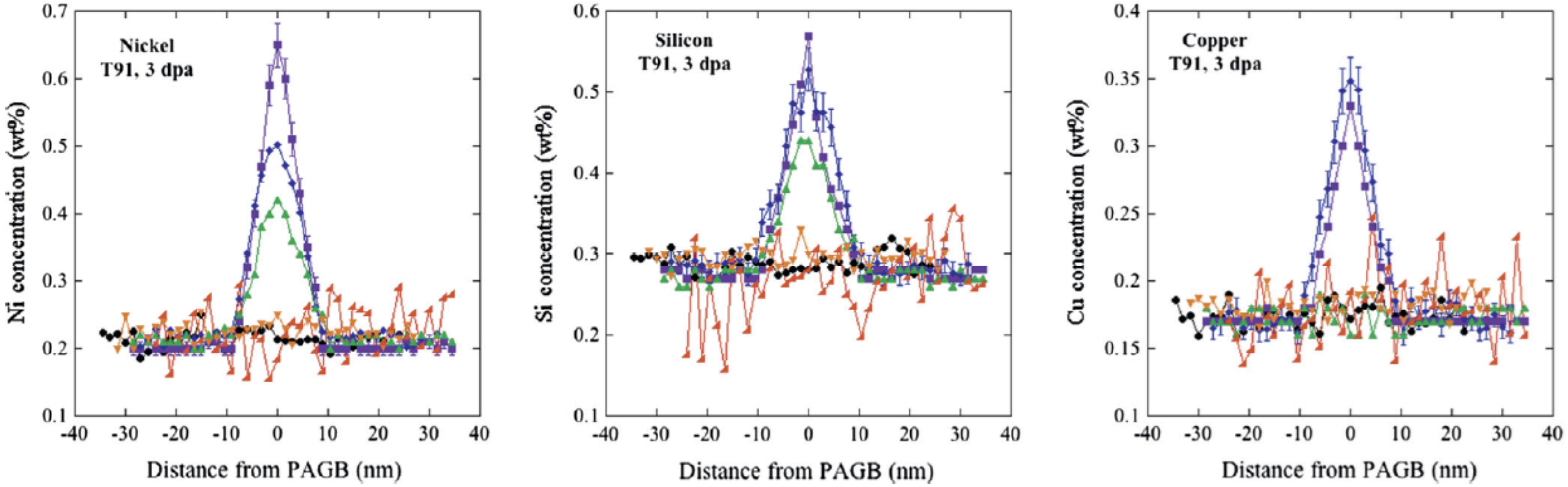
Enrichment of solute atoms at defect sinks (grain boundaries, dislocations, precipitates).





J.P. Wharry, G.S. Was, JNM 442 (2013)
Systematic experimental investigation of RIS in several F/M alloys at low temperature.

- Concentrated in Cr, dilute in Ni, Si, Cu.
- Enrichment enhanced by low temperature.
- Cr switch-over at ≈680°C.



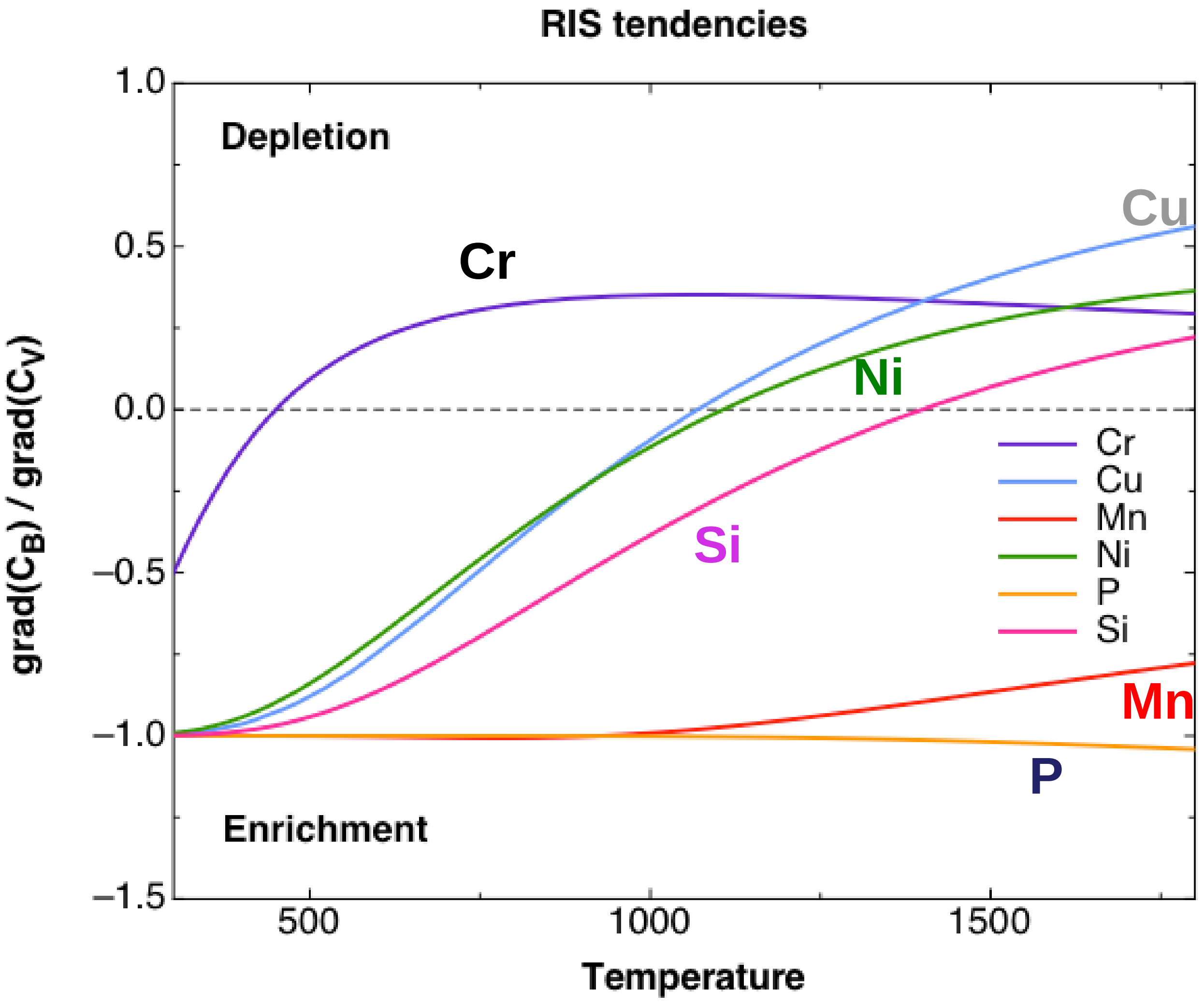
RIS tendencies in dilute alloys

- Enrichment at reactor temperatures for **all solutes**, due to vacancy drag.

- Enriching tendency strongly enhanced by interstitial transport for P and Mn.

- Switch-over T for Cr at 220 °C.

- Rate theory needed for quantitative assessment.



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Embrittlement in dilute ferritic alloys

- Theoretical toolkit developed in collaboration with CEA for correlated diffusion

- Very flexible and general method, applicable to many sorts of crystal structures and migrating objects (defect clusters, foreign interstitials, etc..).

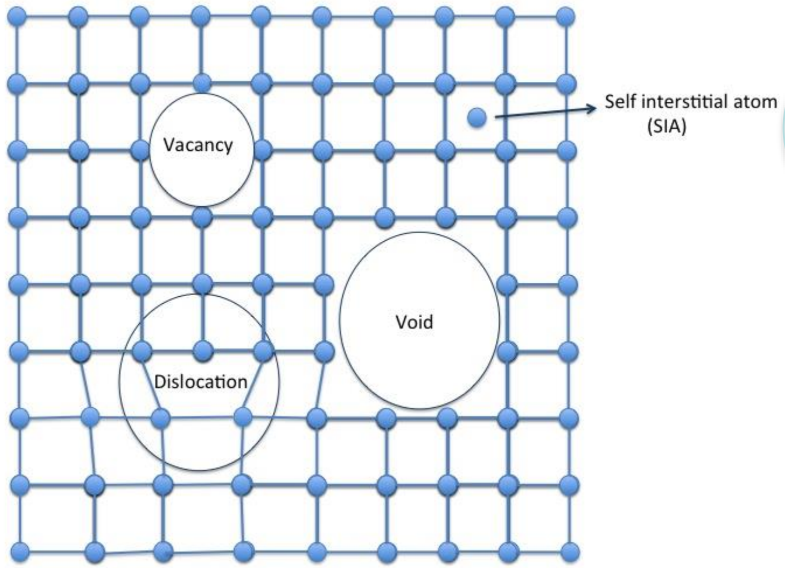
- Exact transport coefficients are calculated through a mean field method by making use of accurate first principle calculations.

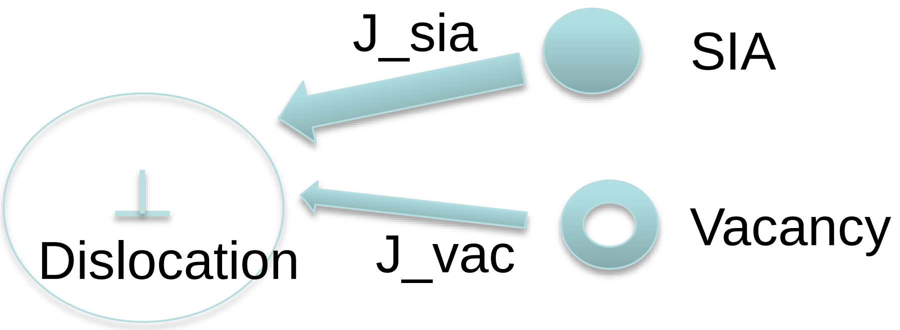
- Main findings
    a) Vacancy drag on all solutes but Cr, enhanced by low temperatures.
    b) Interstitial transport for Cr, P, Mn – not for Si, Cu, Ni.
    c) Vacancy-driven diffusion for Si, Cu, (Ni); interstitial-driven for P, Mn; both for Cr.
    d) Enrichment of solutes at grain boundaries and dislocations.

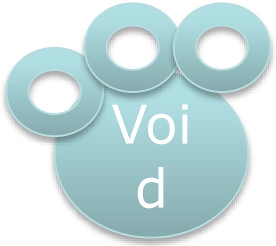
- Solid theoretical modelling of mechanisms for embrittling nanofeature formation in RPV steels.

- To be applied to study also irradiation creep in these alloys!

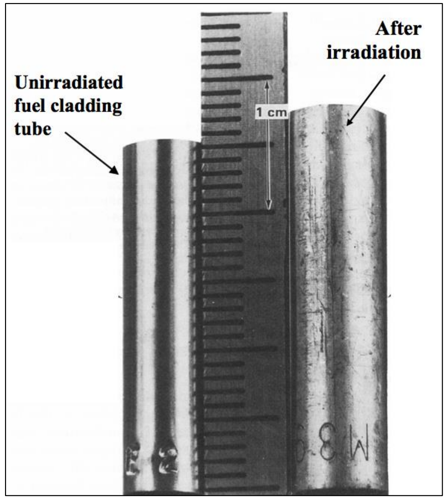
3 – Swelling in fcc and bcc materials







CW316 at 533°C to a fluence of 1.5e23 n/m^2 in the EBR-II.



Void swelling

- Standard rate theory model (dislocation bias)
- Production bias model (production bias, dislocation bias)

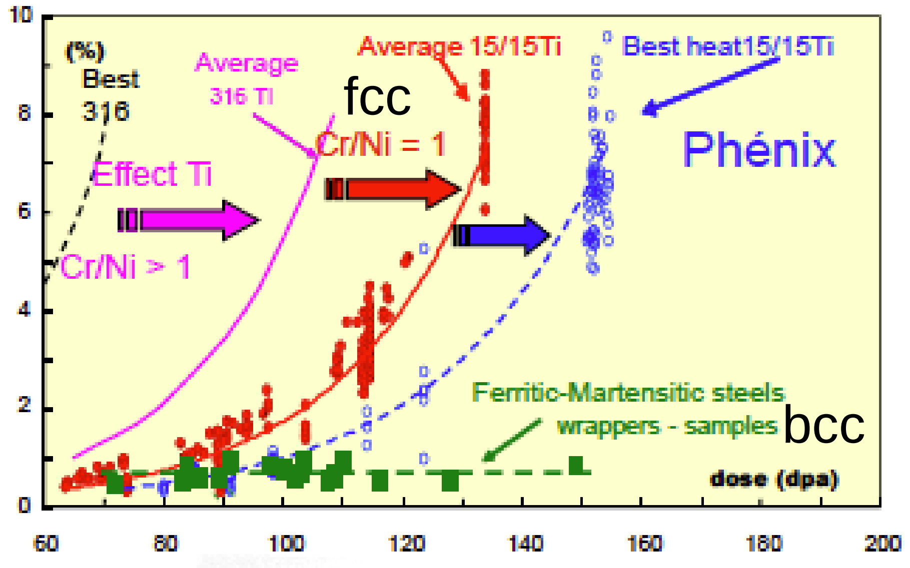
The bias gives rise to a vacancy supersaturation that drives the swelling of the material!

Swelling in fcc and bcc materials

An atomistic description is vital to understand the bias of SIA over vacancy absorption at dislocations

The dislocation bias drives swelling

Fcc and bcc metals behave quite differently – one important revelation here: negative bias of screw dislocations in bcc Fe, positive of edge dislocations!



Materials for energy: Studies at Reactor Physics, KTH

We model diffusion and radiation damage of different kind of material classes

A large range of phenomena in nuclear materials are diffusion controlled

Further studies include:

- Gamma induced damage in final repository canisters
- Radiation stability of ODS (Oxide Dispersion Strengthened) alloys
- Residual resistivity of defects in metals and alloys
- The primary damage state
- Dynamic first principles calculations of threshold damage energies
- Solute effects in dilute and concentrated alloys
- Spin photovoltaics... and much more!

Key publications:

- P. Olsson *et al*, J. Nucl. Mater. 321 (2003) 84.
- P. Olsson *et al*, Phys. Rev. B 72 (2005) 214119.
- P. Olsson, C. Domain and J. Wallenius, Phys. Rev. B 75 (2007) 014110.
- D.A. Terentyev *et al*, Phys. Rev. Lett. 100 (2008) 145503.
- P. Olsson, C. Domain and J.-F. Guillemoles, Phys. Rev. Lett. 102 (2009) 227204.
- J. Vidal *et al*, Phys. Rev. Lett. 104 (2010) 056401.
- P. Olsson, T.P.C. Klaver and C. Domain, Phys. Rev. B 81 (2010) 054102.
- Z. Chang *et al*, J. Nucl. Mater. 441 (2013) 357.
- A. Claisse, P. Olsson, Nucl. Instr. Meth. B 303 (2013) 18.
- L. Messina *et al.*, Phys. Rev. B 90 (2014) 104203.

"Genius is one percent inspiration and ninety-nine percent perspiration."
- Thomas A. Edison

For special attention of David Clark

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Summer Course:

Elements of the Back-end of the Nuclear Fuel Cycle: Geological Storage of Nuclear Spent Fuel

Organizers

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nova CENTER FOR UNIVERSITY STUDIES, RESEARCH AND DEVELOPMENT

Linnæus University

2 weeks in June 2015 for 30 international students/experts.

The key cooperating: universities; **KTH** and **Linneus University** together with Nova Center for University Studies, Research and Development and Swedish Nuclear Fuel and Waste Management Company (SKB).

Summer Course is accredited to KTH: SH262V

7.5 ECTS (credits)

Svensk Kärnbränslehantering AB

Swedish Nuclear Fuel and Waste Management Co

Cooperating universities:

On waiting list: **KAIST, University of Kyoto**

KTH VETENSKAP OCH KONST
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Linnæus University

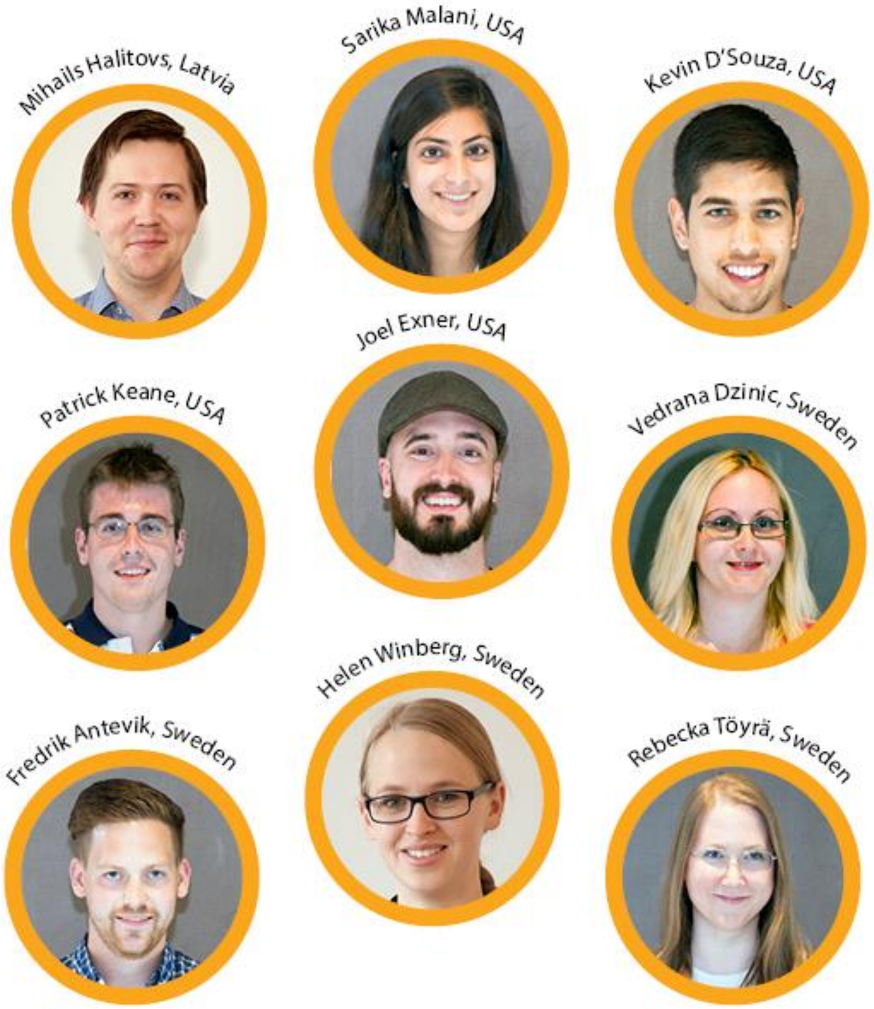
nova CENTER FOR UNIVERSITY STUDIES, RESEARCH AND DEVELOPMENT

EMINE European Master in Innovation in Nuclear Energy

KTH ROYAL INSTITUTE OF TECHNOLOGY

SKB

Students



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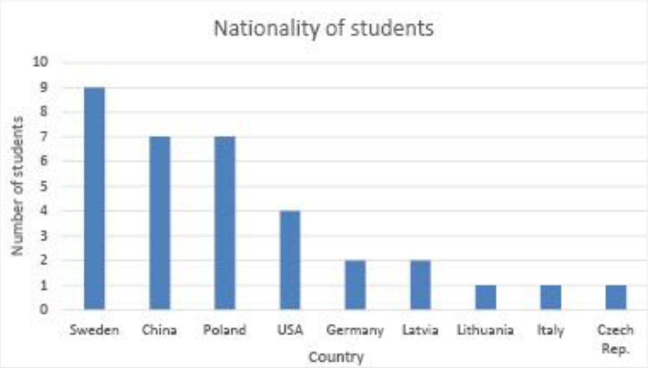
Senior Scientists



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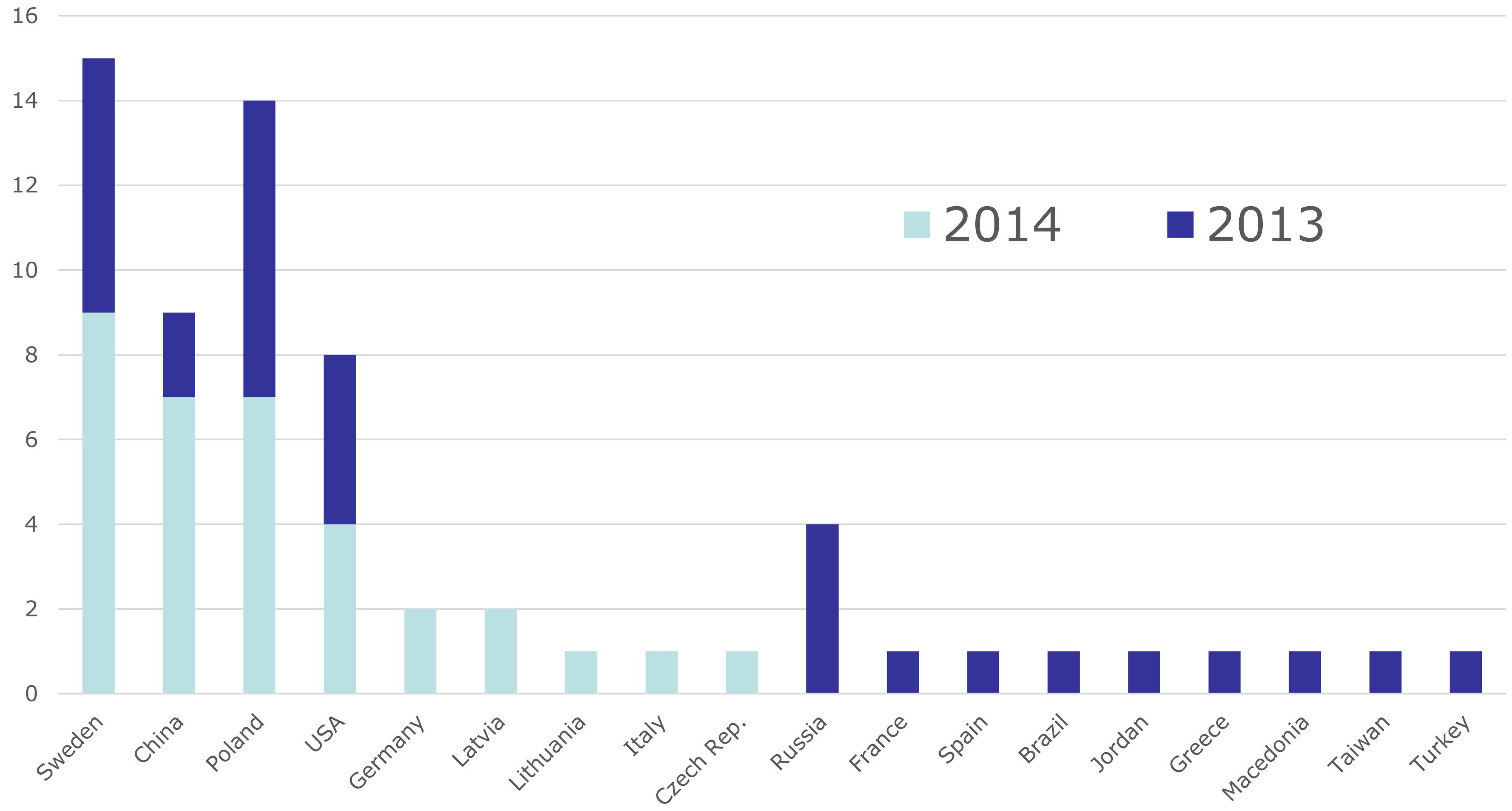
Nationality of the students



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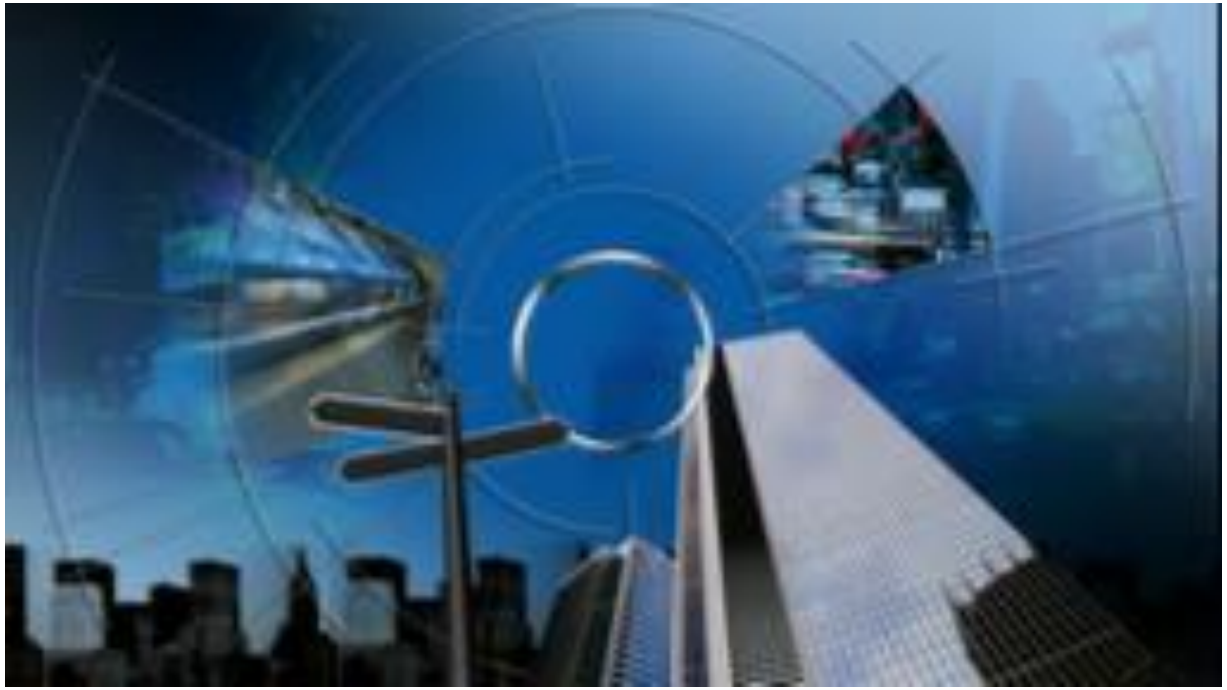
Extensive use of Oskarshamn facillities:

- Äspö Hard Rock Laboratory and field studies
- CLAB – Interim Storage
- Canister Lab
- Reactor visit

VISIT TO CLAB



Exploring Äspö Hard Rock Laboratory with

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Lecturers

Family Name	Name	Photo	Lecture sample
Kozlowski	Tomasz		
Roy	William		
ZHOU	ZHIWEI		
Claesson	Tommy		

Family Name	Name	Photo	Lecture sample
Morosini	Mansueto		
Simeonov	Assen		
Sigurdsson	Oscar		
Luterkort	David		
Åström	Mats		

Lecturers

Family Name	Name	Photo	Lecture sample
Dopson	Mark		
Stenberg	Leif		
Karlsson	Mathias		
Alakangas	Linda		

Family Name	Name	Photo	Lecture sample
Hultgren	Peter		
Rockström	Anna		

Student´s Assignments

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Seven different assignments including:

Prepare a program of the informational meetings with local communities of relevance for a location of the geological storage of spent nuclear fuel.

Prepare and present a 10 minutes presentation for the group presentations June 18-19.

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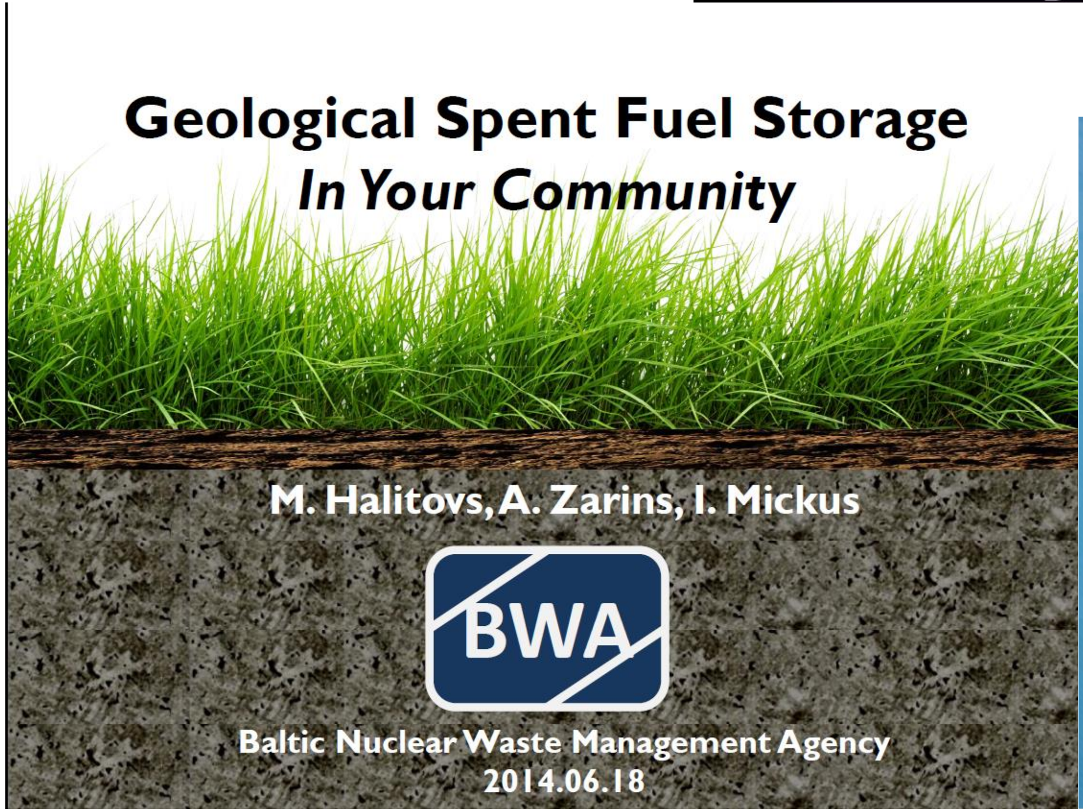
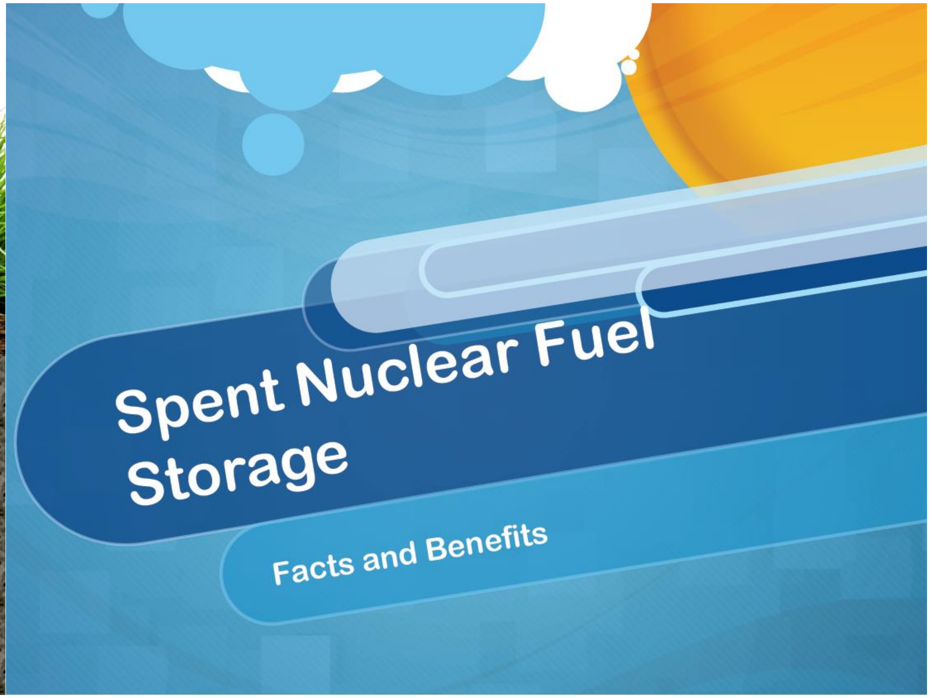
Management Solution and Safety

- Deep below surface in solid bedrock
  - Tunnel system
- Safety barriers
  - Copper canister
  - Bentonite clay
  - Granitic bedrock
- Conservative methods
  - Authority revision
  - Allowed to withdraw at anytime

Who are we?

- Lumadi is a national company, which processes and stores high level radioactive wastes.
- We currently have an interim storage facility, which cools the fuel from the nuclear power plants.





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CERTIFICATE OF COMPLETION

Vedrana Dzinic, Sweden

Vedrana Dzinic, Sweden

has completed the Summer Course 2014 "Elements of the Back-end of the Nuclear Fuel Cycle: Geological Storage of Spent Nuclear Fuel" - Master level, 7.5 ECTS.
This Summer Course was organised jointly by the Royal Institute of Technology and Linnaeus University, European Master inInnovative Nuclear Technology - EMINE with support of Nova-Oskarshamn and SKB.

Oskarshamn, Sweden

19/06/2014

Waclaw Gudowski, Professor, KTH

Tommy Claesson, Docent, Linnaeus University

Student’s Assessment:

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Course Evaluation Questionnaire

Course = Elements of the Back-end of the nuclear fuel cycle: Geological Storage of Spent Nuclear Fuel - SH262V

Code = SH262V

Year - 2014

Student’s feedback

95% of students responded!!

Grading - 7 levels as in the Bologna agreement:

7 = A = Excellent;
6 = B = Very Good;
5 = C = Good;
4 = D = Average;
3 = E = Below Average;
2 = Fx = Poor.
1 = F = Very Poor.

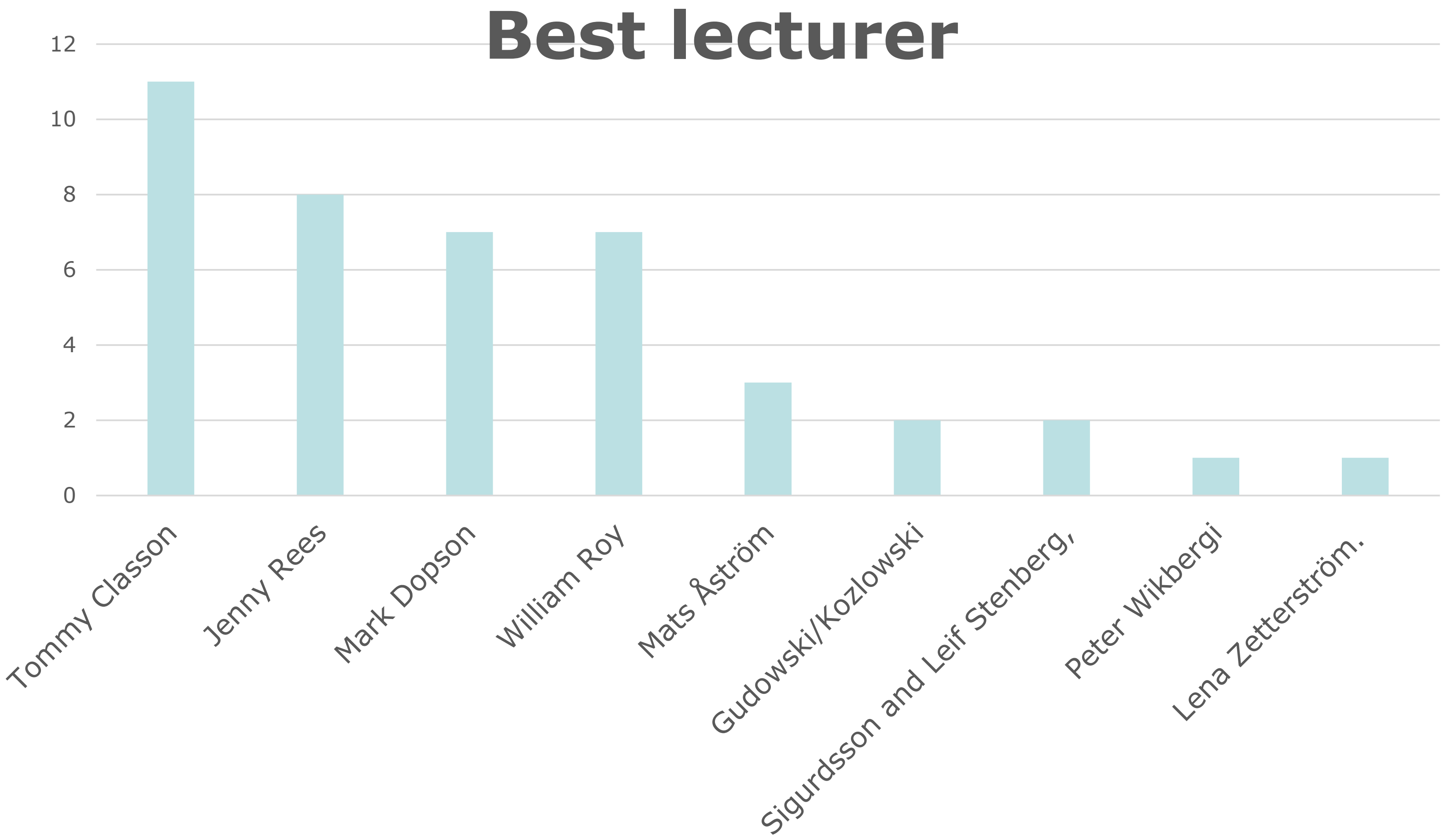
21 questions rated from 1-7

5 descriptive questions:

22	The best lecture:
23	Lectures to be improved:
24	Are there issues or aspects that were lacking in the course (e.g. matters that were not included at all)
25	Improvement of the course - give verbal suggestions/advice/ comments
26	Your reasons for joining the course – summarize in a few words why you wanted to develop your competence in the topics of the course.

Student’s Assessment:

All over average: 6,50 (excellent)



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Options for a developing co-operation LANL-KTH-NORDITA

From KTH to LANL

Investment in students:

- Undergraduate level:
  - 3-4 week projects at LANL for undergraduate students in Modern Physics. 3-4 students per year
  - MSc level - common MSc thesis projects:
    - 6 months KTH-LANL MSc thesis project at LANL. 2-4 students per year.
- PhD level:
  - Common PhD students – model: 1 year at LANL, 2 years at KTH, or opposite
  - Question: funding model
- Post-doc level:
  - Balanced post-doc program in nuclear technology + more
  - Question: funding model

Options for a developing co-operation LANL-KTH- NORDITA

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From LANL to KTH and back

Fuel Cycle Cooperation:

- Summer Course in Oskarshamn
  - We can invite annualy 3-6 LANL experts either as trainees or lecturers (David, you are welcome already this year for a guest lecture on US program)
  - We can offer this co-operation with ”unlimited” research extension possibilities for an entire DOE nuclear waste/spent fuel disposal programs.
  - **A vision:** Sweden-US cooperation on entire nuclear fuel cycle: from advanced front end to safe, secure and socially acceptable back-end of the NFC.
  - Economy?? Different viable options are visible on a horison. A small working group?
- Thematic lab-to-lab (project-to-project) cooperation:
  - Study visits and synchronisation of research on:
    - NFC – new, accident tollerant and economical nuclear fuels and fuel cycles.
      - **Revival of ATW/ADS activities?**
    - Nuclear power safety – new materials of relevance for nuclear power safety: sacrificial materials, heavy metal coolants etc.

Options for a developing co-operation LANL-KTH- NORDITA

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From LANL to KTH and back

LANL-KTH-NORDITA Seminar and Lecture Program:

- KTH-NORDITA-LANL run a dedicated seminar program in Stockholm (involving academies of science) on Frontiers of Science and Technology
  - Twice (once??) a year 2-3 day seminar program on different topics. We start with W. Zurek in September this year. Establishing a program committee ??

Guest lectures of LANL experts for Master and PhD Programs at KTH on selected topics.

More to come……

Thank you for your attention!